JETSCAPE Annual Report 2016 – 2017

(*text in italics is institution specific*, **Bold face are questions from NSF**)

Tab: Accomplishments

Accomplishments - What was done? What was learned?

Box1: What are the major goals of the project?

The primary goal of the JETSCAPE collaboration is to design and deploy an overarching software framework that can be used by the entire community of theorists and experimentalists to program, simulate and study complete events that can reproduce every aspect of high-energy heavy-ion collisions. The collaboration will,

1) Design and implement a C++ framework which encompasses all currently known aspects of high energy heavy-ion collisions, from large symmetric systems such as Pb-Pb to extremely asymmetric collisions such as p-Pb (and eventually e-A collisions). The framework must be able to incorporate new physics insights and provide a basis for systematic study of new hypotheses.

2) Develop standard routines for each of the modules within the framework and make these available as part of the release

3) Develop new physics capability through new software routines, such as a multi-stage jet modification generator, where the interaction of the jet with the medium varies at the parton level depending on its properties.

4) Develop new physics capability such as simultaneous and interacting execution of jet propagation and fluid evolution through new software routines.

5) Develop new software based modeling capability involving hadronization of jets in the presence of a medium.

6) Accelerate computationally intensive portions of code by porting to GPUs, and develop dual versions of release for running on both hybrid and non-hybrid architectures.

7) Develop new statistical emulation tools to sample the multidimensional phase space of input parameters by comparison to corresponding data sets.

8) To train the emulation routines on ever more sophisticated event generators in comparison with continually improving data sets.

9) Develop bridges between the event generator framework and detector analysis tools to carry out seamless comparisons between theoretical simulations and experimental data.

10) Carry out extensive phenomenological comparisons between each stage of the statistically improved event generator and experimental data.

Box 2: What was accomplished under these goals (you must provide information for at least one of the 4 categories below)?

Major Activities:

The activities of the collaboration have been divided into 3 major parts as codified in the objectives of the three working groups of the collaboration:

The software design WG (COMP): this is the largest of the three working groups and is tasked with development of the major software deliverables of the collaboration.

The Physics Modeling WG (PHYS): Several of the deliverables of the collaboration involve physics processes that have never been realized in an event generator set up. The PHYS WG is tasked with carrying out ground-breaking simulations of these novel processes, to discover new algorithms that will lead to efficient simulations of these processes, and to establish bench marks for the results of such simulations in simplified systems.

The Statistics and Data analysis WG (STAT): Tasked with developing continually more extensive Gaussian emulation routines to carry out statistical studies of comparisons between the simulations and experimental data. Members of STAT will liaise with experimental collaborations to obtain curated data and the covariance between various observables.

In the first annual reporting period, the following objectives were achieved by the COMP group:

A software framework was developed that allows a user to incorporate

a) The simulation of the initial state of the collision of two nuclei yielding the soft density distribution that becomes an input to the fluid dynamical simulation.

b) The generation of the binary collision density profile which is sampled to generate hard jets.

c) A routine that calls a p-p event generator such as PYTHIA to generate the hard collisions and yield final state partons.

d) A routine to call and run a fluid dynamical simulation taking input from the initial state density distribution and ending at hadronization followed by freezeout.

e) A set of routines that carry out an integrated set of calls to a series of jet modification routines, with varying levels of detail regarding the resolution of the medium by the jet. These routines describe the multi-stage modification of the jet shower.

f) Routines that carry out the hadronization of the partons, near the phase transition hyper-surface, in the hadronic phase and in the vacuum.

In the first annual reporting period, the following objectives were achieved by the PHYS group:

a) Development of the JET-patch codes to set up bench marks for the eventual JETSCAPE production codes.

b) Creation of the first Multi-State Monte Carlo event generator that combines several different event generators, within one overarching generator, where transitions between one model and the next occur on a parton-by-parton level.

c) Set up of new routines to describe the hadronization of the jet in the presence of a hadronizing medium, followed by a hadronic medium, and eventually in vacuum.

In the first annual reporting period, the following objectives were achieved by the STAT group:

a) Education of the broader collaboration on the basics of Bayesian statistical analysis

b) Commencing a pilot project: a simple model for the calculation of di-jet asymmetries is utilized to generate histograms for the di-jet asymmetry observable Aj. This model data is now being used to train a set of Gaussian Process Emulators specifically tuned to be robust regarding the specific properties of the Aj histogram (a peaked distribution with subsequent rapid fall-off to zero).

c) Setting up a complete statistical analysis, utilizing a Linearized Boltzmann Transport (LBT) model for the calculation of leading particle energy-loss, in particular the nuclear modification factor R_{AA} and elliptic flow coefficient v_2 as a function of transverse momentum. In this study, only two parameters related to the scale, temperature and momentum-dependence of the QCD running coupling constant are varied.

Box 3: Specific Objectives:

In year 1 the focus of the Wayne state group in collaboration with the PHYS-WG, was on developing a unified theoretical approach for medium-modified parton showers in relativistic heavy-ion collisions. Jets are produced via hard scatterings at the primordial stage of heavy-ion collisions and therefore start with high virtuality and high energy. As the partons in a jet split into more partons, they lose virtuality at a far greater rate than energy, and spend a portion of their path in the medium with low virtuality that is comparable to the medium (thermal) scale while their energy may still be high. Medium-modified parton showers will continue for these energetic partons until their energy drops to the thermal scale, as well when they start interacting strongly with medium. The underlying physics for jet-medium interaction is different at these various virtuality and energy scales. To date, no calculation or simulation of jet modification has accounted for these different phases of the jet interaction with the medium. All previous efforts have *used a single formalism and applied it to the entire space-time history of the jet. The WSU group in collaboration with the PHYS-WG is working on developing a unified framework in which through the full evolution history of jet, its different stages are properly treated with different physics formalisms and these different formalisms may smoothly transit between each other at the boundary of the different stages. This will be one of the most important physics input into the JETSCAPE framework that simulates the entire temporal evolution of heavy-ion collisions.*

The PHYS-WG has completed its Step 1 task over the past 6 months: combining MATTER and MARTINI/LBT in a static medium. MATTER, based on the higher-twist energy loss formalism, is a well developed event generator that simulates parton showers at high virtuality scale. MARTINI, based on the AMY energy loss formalism, and LBT, based on a derivative of the higher twist energy loss formalism, are two different event generators that treat parton showers at low virtuality but high energy equally well. We have designed both fixed and dynamical virtuality separations scales between MATTER and MARTINI/LBT and combined these different models into a unified approach for parton showers. Within a static medium, we have investigated the relative weights of the different energy loss schemes for the medium modifications experienced by the jet by varying the parton energy, medium length and virtuality separation scale. Our results have been documented and will serve as an important benchmark for the future physics development within JETSCAPE. A majority of this work was carried out in collaboration with the group at McGill and Berkeley as part of the PHYS WG.

Box 4: Significant results:

Algorithms: New algorithms that combine multiple event generators at a parton-by-parton level were designed, and tested in the patch code. Results from this test have been described in a paper that is currently undergoing collaboration review, and will be published shortly. The current version is attached with this report.

Data Structures: An entirely new approach employing graph theory with nodes for vertices and edges for partons was deployed to store, search and study parton showers. These routines now form the core of the framework that generates parton showers in medium and vacuum. An internal note documenting this framework is attached with this report.

Box 5: Key outcomes or other achievements:

The current implementation of the JETSCAPE (Core) Framework is a task-based C++ Object-Oriented (OO) framework with emphasis, from the software design perspective, on minimizing external library dependencies, using C++11 smart pointers consistently, and adhering to a strict data encapsulation paradigm. The task-based approach allows maximum flexibility for future extensions of physics modules as our understanding of partonic energy loss utilizing JETSCAPE evolves, as well as simplifies and clearly defines a straightforward interface for developers. Furthermore, expressing the physics modules as tasks allows us, in the near future, to parallelize the framework with minimum overhead and redesign of the core code. The "communication" between different modules is achieved by utilizing a Signal/Slot approach (inspired by Trolltech's Qt). The primary advantage of this approach, besides the direct mapping between the "logical" physics setup of the problem and the task-based approach, is that it allows a much cleaner (encapsulated) and well-defined communication interface across modules. Furthermore, signal/slots are a straightforward and elegant solution to interface and decide, based on physics criteria, which physics modules are responsible to perform the needed calculations. In addition, this approach is naturally suited to simplifying the concurrency problem in later JETSCAPE implementations with emphasis on running the jets energy loss and hydro in parallel.

A graph structure was chosen as the data format for the parton shower. The graph structure is well suited for providing maximum flexibility for further physics development, as well as providing an interesting computational problem for the computer scientists toward efficiently extending the graph structures (multi-layered with different physics quantities and interactions) and traverse algorithms for the specific physics needs.

Box 6: What opportunities for training and professional development has the project provided?

List the work of students and postdocs in your group. How has working for JETSCAPE improved their training, e.g., *Starting in July 2016, At Wayne State, the JETSCAPE award has supported the research of 2 graduate students (A. Kumar, C. Sirimanna) and currently two postdoctoral fellows (Dr. S. Cao, Dr. D. Pablos). One more postdoctoral fellow (Dr. K. Kauder) is set to be hired in May, and a research assistant professor (Dr. E. Khalaj) is set to be hired in June of 2017.*

Both students are currently being trained in the design of the C++ code along with a suitable framework for extending this code, working within a large collaborative process. The current postdoctoral fellow (Dr. S. Cao) has been assigned a leadership role as convener of the PHYS working group, where he leads a team of several other collaborators in designing algorithms for the most efficient multi-stage event generators.

It is anticipated that Dr. K. Kauder will replace Prof. L. Schwiebert as convener of the COMP group, and will be replaced after a year by Dr. E. Khalaj.

How have the results been disseminated to communities of interest?

The JETSCAPE collaboration has engaged a wide cross section of the heavy-ion community within its external associates. Several of these individuals attend regular meetings where the framework is being designed. Some of them are actively engaged in the design of extra functionality to be included with the upcoming release. Being part of the development induces a sense of ownership among the community members and is expected to ease adoption of the framework.

New algorithms to be incorporated within the framework are first tested within a patch code framework made up of older codes of the JET collaboration. The benchmark results obtained will be published prior to their incorporation with the JETSCAPE distribution.

Members of the collaboration have given talks at major international conferences (e.g., Quark Matter), at experimental collaboration meetings (e.g., STAR collaboration meeting), and at invited seminars and colloquia where the work of the collaboration was advertised.

What do you plan to do during the next reporting period to accomplish the goals?

The COMP WG will continue to incorporate more physics modules within the framework. It will continue to test with a variety of different physics implementations to test the functionality of the framework.

The STAT group will work in collaboration with the COMP group to design new Gaussian process emulators for the full simulations, to obtain experimental data with covariance errors, and carry out comprehensive statistical comparisons between theoretical predictions and experimental data.

The PHYS and COMP groups will work in tandem in year 2 to carry out the incorporation of concurrent running of jet propagation with energy loss and hydrodynamics with energy deposition. This will require several advancements to the framework and a more accelerated setup to handle the

The collaboration will continue to strive to engage an even wider community in the process of design and development of the software. Beta versions of the software will be distributed within the associate community. We will work closely with users to facilitate the incorporation of their software into the JETSCAPE framework. This will provide direct feedback on how easily adapted our framework is for users. When these efforts indicate cases where code refactoring or interface changes are required, we will generalize the framework accordingly.

The collaboration is planning a winter school for graduate students across the US and a workshop to highlight the developed framework and hasten its deployment across the heavy-ion community. These events are planned for early January 2018.

Products - What has the project produced?

List any papers that were written with JETSCAPE funding.

What is the impact on the development of the principal discipline(s) of the project?

The research of the three working groups of the JETSCAPE collaboration introduces an entirely different methodology in how theoretical calculations are simulated and compared to experimental data: Instead of approximating a theoretical calculation to the point where a numerical simulation can be motivated and carried out, a general computational framework for heavy-ion collisions is designed. This includes an initial state, leading to the generation of an initial condition for fluid dynamical simulations and hard partons, which will eventually become jets.

The portion of the code which describes the propagation and modification of jets is made of partons and vertices. To be included in this framework, any theoretical calculation will have to approximate and yield the properties of these partons and vertices. Quantities such as the starting four-momentum of the partons, the drag and diffusion experienced by the partons between vertices will have to incorporated as an event-by-event shift sampled from a theoretical distribution. Most importantly, the theoretical calculation will have to clearly delineate the range of four-momenta of a parton over which that particular theory is applicable. It will have to predict the locations of the vertices in space-time and also the number of active partons at that vertex.

In this way, the framework enhances a theoretical formalism by combining it with state-of-the-art components, which provide the source, background and outcome of a particular section of a heavy-ion collision, which is sensitive to the theory in question. It also constrains the theoretical formalism by requiring boundaries within which the theory is applicable and requiring it to interface with the remainder of the simulation via a generic interface. This forces competing theories on to a level playing field, simulating them only within the region of applicability and comparing them to experimental data within a simulation where all other components are exactly the same.

Beyond the obvious impact on physics, the JETSCAPE project enhances the interaction between physics, computer science and statistics. In order to emulate the entire the system, with a variety of variable theories, the Gaussian process emulation framework will have to enhanced to a point where it can decide between competing theories and not just identify the best fit parameters, and correlations between them.

What is the impact on other disciplines?

It is envisioned that the work of the JETSCAPE collaboration in setting up a framework that be used to discern between different theories encapsulated within sophisticated phenomenology will find applications in a variety of different fields such as astrophysics, nuclear stockpile stewardship, and climate science.

What is the impact on the development of human resources?

The JETSCAPE collaboration currently funds the dissertation research of 4 graduate students at Duke, OSU and TAMU, and partially funds the research of 4 other graduate students at MIT and WSU. It funds either wholly or in part, the research of 5-6 postdoctoral fellows. It impacts the research of an equivalent number of postdoctoral fellows and graduate students at JETSCAPE institutions who are not directly funded by the grant. It also influences the training of several other students and postdoctoral fellows, at institutions of JETSCAPE associates, and funds the research of a research assistant professor in computer science at WSU.

In so doing, the JETSCAPE collaboration influences a considerable portion of the future workforce in theoretical/computational nuclear physics. It also influences a non-negligible portion of the experimental nuclear physics workforce, especially those involved in the analysis of experimental data.

What is the impact on physical resources that form infrastructure?

While the work of the JETSCAPE collaboration in year 1 is not expected to produce an impact on physical resources, in time, it is expected to influence the design of the Future S-PHENIX detector. Several experimentalists working within the collaboration and as associates are associated with the S-PHENIX project.

As the framework becomes more generalized, it is expected to play a major role in the experimental design of the future EIC detectors.

What is the impact on institutional resources that form infrastructure?

The JETSCAPE collaboration has had a major effect on Wayne State institutional resources in particular those related to HPC. There is now a commitment from the university to invest in computational resources to serve the needs of the collaboration. Future MRI proposals are currently being envisioned based on JETSCAPE in combination with several other SSE and computationally intensive research groups within the university.

What is the impact on information resources that form infrastructure?

What is the impact on technology transfer?

What is the impact on society beyond science and technology?